Amendments to the Claims:

1. (Currently Amended). A method for calculating the similarity of at least one chemical compound to at least one chemical probe, comprising the steps of:

(a) utilizing at least one chemical descriptor for each of a plurality of compounds, each descriptor comprising a row of a molecule-descriptor matrix X;

(b) representing each compound as a column of the molecule-descriptor matrix, the entries of the molecule-descriptor matrix comprising a frequency of each descriptor for each compound;

(c) performing a partial singular value decomposition (SVD) of the molecule-descriptor matrix to produce resultant matrices P, Σ and Q^T, comprising:

generating the resultant matrices P, Σ and Q^T, such that molecule-descriptor matrix $X = P\Sigma Q^T$, wherein:

P is a mxr matrix, called the left singular matrix, where r is the rank of X, and its columns are eigenvectors of XX^T corresponding to nonzero eigenvalues;

Q is a nxr matrix, called the right singular matrix, whose columns are eigenvectors of X^TX corresponding to the nonzero eigenvalues; and

Σ is a rxr diagonal matrix whose nonzero elements, $\sigma_1, \sigma_2, \ldots, \sigma_r$ called singular values, are the square roots of the nonzero eigenvalues and have the property that $\sigma_1 \geq \sigma_2 \geq \ldots \geq \sigma_r$;

(d) creating a chemical probe descriptor matrix for the at least one chemical probe, the entries of the chemical probe descriptor matrix comprising a frequency of each descriptor for each chemical probe;

(e) ~~using at least one of the resultant matrices to calculate~~ calculating the similarity

between the at least one chemical probe and at least one compound of the molecule descriptor matrix by:

generating a reduced dimension approximation of X of rank k, defined as $X_k = P_k \Sigma_k Q^T_k$, wherein $k < r$ and Σ_k is an identity matrix;

generating a pseudo-object, denoted as O_F, where $O_F = F^T P_k \Sigma^{-1}_k$, and where F is a molecule-descriptor vector for the at least one chemical probe; and

taking a dot product of O_F with one or more columns of Q^T_k respectively corresponding to the at least one compound; and

(f) providing an output indicating the similarity between the at least one chemical probe and the at least one compound.

2. (Previously Presented). The method as recited in claim 1, wherein each of the at least one chemical descriptors comprise at least one of an atom pair descriptor and a topological torsion descriptor.

3 - 29. (Cancelled).